

Propagation of the discontinuities of the quantum wave function along the classical trajectories for 1/2-spin particles

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We address the propagation of spin discontinuities for a 1/2-spin particle obeying Dirac equation with scalar potentials. We find an explicit spin-transport law for the case of the Dirac oscillator. In the general case we follow an eikonal asymptotic approach after the wave equation. Throughout we establish as many parallels as possible with the equivalent situation for the electromagnetic field.

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I. INTRODUCTION

In the theory of light is well known the deep relationship between electromagnetic and geometrical optics. Usually, geometrical optics is considered as an approximation valid in the limit of short wavelengths [1, 2]. On the other hand, another radically different point view is possible: the light rays of geometrical optics is the exact way in which the surfaces of field discontinuity propagate, for all wavelengths [3, 4]. In this context, a natural question appear: what happens with the polarization of the particle across this propagation? A simple calculus shows a coupling between the rays of the light, the gradient of the refraction index, and the field itself; consequently, it can be proved the ellipse of polarization just rotates along the propagation, but always keeps its form [3, 4]. It is a remarkable phenomenon that the polarization transformation is of purely geometrical origin since it depends only on the form of the trajectory, becoming an example of topological dynamics.

Exactly the same philosophy can be applied to the quantum mechanics; consequently, classical mechanics is either an approximation for short values of Planck constant, this is, the Wentzel-Kramers-Brillouin (WKB) methods [5], or the exact way for the propagations of the discontinuities of the wave function, as it was proved in the last decade for spinless particles [6]. More specifically, it has been shown that the surfaces of discontinuity of the quantum wave function (relativistic and non relativistic) propagate exactly following the classical trajectories. This is because such surfaces must be a solution of the corresponding classical Hamilton-Jacobi equation [7].

In this work we address what happens with the spin state of a 1/2-spin particle when its vectorial wave function is transported along the classical trajectories of a discontinuity, in the same sense we know about the transport of photon polarization. To this end we mimic the

electromagnetic case as far as possible, focusing on particles experiencing scalar potentials, and on time-harmonic solutions since this allows to express the Dirac equation where all terms present a derivative in a suitable way to apply the divergence theorem [6].

We are able to complete this program for the evolution of the spin along the classical trajectories for the wave-function discontinuities of a particular case: the Dirac oscillator [8]. Otherwise, in the general case the main obstacle lies in the fact that the Hamilton-Jacobi equation for the discontinuity does not include a specific term coupling spin and trajectory. Thus the divergence theorem only says that the discontinuity behaves as a locally free particle with position-dependent parameters. So at any point any spin state is possible for the quantum-state discontinuity.

To avoid this obstacle in the general case we take advantage of the formal similarity between Maxwell's and Dirac's theories as recalled in Appendix A, in particular regarding the equivalence between eikonal and WKB approximations. A priori, these approximation methods are different and independent from the exact propagation of discontinuities. However, in the short-wavelength limit we may consider that the phase of the quantum wave function becomes effectively discontinuous at every point of the space. In fact, this equivalence is supported by the coincidence of the equation for the discontinuity (the Hamilton-Jacobi equation) with the leading terms of the eikonal and WKB approximations.

Moreover, we show that this asymptotic approach is fully consistent with the exact result obtained for the Dirac oscillator and previous relativistic WKB derivations [5]. In this regard our approach turns out to be quite simple while throughout preserving a direct parallel with the electromagnetic case.

II. DIRAC OSCILLATOR

The Dirac oscillator is a simple model for a relativistic isotropic oscillator of frequency ω and mass m , that preserves the fully linear character of the Dirac equation

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[8]

$$i\hbar\dot{\Psi} = c(\mathbf{p} \cdot \boldsymbol{\alpha} - im\omega \mathbf{x} \cdot \boldsymbol{\alpha}\beta + mc\beta) \Psi, \quad (2.1)$$

where $\mathbf{p} = -i\hbar\nabla$, $\boldsymbol{\alpha}$ and β are the 4×4 matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad (2.2)$$

$\boldsymbol{\sigma}$ are the three Pauli matrices, I the 2×2 identity, and the spinorial four-dimensional wave function Ψ depends on the Cartesian coordinates \mathbf{x} and time t . We focus on harmonic wave functions

$$\Psi = \frac{i\hbar}{E} \dot{\Psi}, \quad (2.3)$$

so that Eq. (2.1) can be rewritten as

$$\frac{\partial \Psi}{\partial t} = -c\boldsymbol{\alpha} \cdot \nabla \Psi + \frac{c}{E} \frac{\partial}{\partial t} [(-im\omega \mathbf{x} \cdot \boldsymbol{\alpha}\beta + mc\beta) \Psi]. \quad (2.4)$$

Since all terms have partial derivatives we can apply the divergence theorem as in Ref. [6], leading to

$$[\Psi] \frac{\partial S}{\partial t} = -c\nabla S \cdot \boldsymbol{\alpha} [\Psi] + \frac{c}{E} \frac{\partial S}{\partial t} (-im\omega \mathbf{x} \cdot \boldsymbol{\alpha}\beta + mc\beta) [\Psi], \quad (2.5)$$

where $[\Psi]$ represents the discontinuity of the quantum spinor at the surface of discontinuity $S(\mathbf{x}, t)$.

For the sake of clarity this four-dimensional equation can be split into a pair of two-dimensional equations

$$\begin{aligned} (mc^2 - E) \frac{\partial S}{\partial t} [\phi] &= c(E\nabla S - i\frac{\partial S}{\partial t} m\omega \mathbf{x}) \cdot \boldsymbol{\sigma} [\chi], \\ -(mc^2 + E) \frac{\partial S}{\partial t} [\chi] &= c(E\nabla S + i\frac{\partial S}{\partial t} m\omega \mathbf{x}) \cdot \boldsymbol{\sigma} [\phi], \end{aligned} \quad (2.6)$$

where the two-dimensional spinors ϕ , χ are defined as

$$\Phi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}. \quad (2.7)$$

Using one of the Eqs. (2.6) to remove the discontinuity of the lower spinor $[\chi]$ and using the general relation

$$(\mathbf{A} \cdot \boldsymbol{\sigma})(\mathbf{B} \cdot \boldsymbol{\sigma}) = (\mathbf{A} \cdot \mathbf{B}) I + i(\mathbf{A} \times \mathbf{B}) \cdot \boldsymbol{\sigma}, \quad (2.8)$$

we get a two-dimensional equation for the discontinuity of the upper spinor $[\phi]$

$$\left(\frac{\partial S}{\partial t}\right)^2 (E^2 - m^2 c^4) [\phi] = c^2 \left[E^2 (\nabla S)^2 + \left(\frac{\partial S}{\partial t}\right)^2 m^2 \omega^2 \mathbf{x}^2 + 2mE\omega \frac{\partial S}{\partial t} (\mathbf{x} \times \nabla S) \cdot \boldsymbol{\sigma} \right] [\phi]. \quad (2.9)$$

This equation is of the form

$$\mathbf{b} \cdot \boldsymbol{\sigma} [\phi] = \lambda [\phi], \quad \mathbf{b} \propto \mathbf{x} \times \nabla S, \quad (2.10)$$

where \mathbf{b} and λ are real. Since with $\lambda = \pm|\mathbf{b}|$ we must have

$$\left(\frac{\partial S}{\partial t}\right)^2 \frac{E^2 - m^2 c^4}{E^2 c^2} - (\nabla S)^2 - \frac{1}{E^2} \left(\frac{\partial S}{\partial t}\right)^2 m^2 \omega^2 \mathbf{x}^2 \pm \frac{2m\omega}{E} \frac{\partial S}{\partial t} |\mathbf{x} \times \nabla S| = 0. \quad (2.11)$$

This is the equation that $S(\mathbf{x}, t)$ must satisfy in order to describe a surface of discontinuity for the quantum wave function of a Dirac oscillator. Note that actually there is no sign freedom in Eq. (2.11) since there is no sign ambiguity in Eq. (2.9).

Equation (2.11) can be readily interpreted as the Hamilton-Jacobi for the Dirac oscillator, and its solutions are the corresponding classical trajectories where ∇S is normal to the discontinuity surface and tangent to the trajectory at each point. These trajectories are the same plane ellipses of the standard oscillator since the extra term $\mathbf{x} \times \nabla S$ just depends on the orbital angular momentum that is a constant of the motion.

The key point for our purposes here is that the eigenvalue equation (2.9) singles out a single definite spin state at each point so it explicitly contains how the spin is transported along the classical trajectories. More specifically, the spin state is always an eigenstate of the spin projection along the direction of the orbital angular momentum $\mathbf{x} \times \nabla S$, i. e., normal to the plane where the trajectory is contained. Thus we may say that the spin does not influence on the trajectory while the trajectory forces the spin state. Therefore, it seems that the topological properties of the photon-polarization transport are lost in the 1/2-spin case.

This explicit spin evolution for the discontinuity holds

because of the presence of a strong spin-orbit coupling that is preserved also in the nonrelativistic limit [8]. Nevertheless, the physical system being described is an harmonic oscillator whose potential is scalar.

III. EIKONAL APPROACH

For physical situations with scalar potential other than the Dirac oscillator the divergence theorem does not provide enough information to determine the spin evolution along trajectories. To avoid this obstacle we translate to the quantum domain the same eikonal approach of the electromagnetic field, with particular emphasis in preserving as far as possible the parallelism with the electromagnetic case, in particular regarding its simplicity.

A. Transport equation

Let us address the Dirac equation for a 1/2-spin particle within a scalar field represented by the scalar potential $V(\mathbf{x})$ and time-harmonic wave function

$$[-i\hbar c\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + mc^2\beta + V(\mathbf{x})] \Psi = E\Psi, \quad (3.1)$$

This means we are setting our argument from the point of view of the second-order differential nature of the wave equation. It might be possible to proceed from first-order differential equations in the case of particle coupled to a general electromagnetic field [5]. Instead, in this work we address a more transparent approach just in terms of an arbitrary scalar potential, mimicking as far as possible the electromagnetic situation in isotropic and possibly inhomogeneous media, where light evolution is governed by scalar position-dependent quantities. Going further into this development, we apply the eikonal approximation $\hbar \rightarrow 0$ as an analog of the electromagnetic Eq. (A4), looking for solutions of the form

$$\phi = (\phi_0 + \hbar\phi_1 + \dots) e^{iS/\hbar}, \quad (3.5)$$

where here $S(\mathbf{x}, t) = W(\mathbf{x}) - Et$ is the phase of the wave.

Substituting Eq. (3.5) into Eq. (3.4), we get the fol-

Splitting the four-dimensional spinor Ψ as in Eq. (2.7), the four-dimensional matrix equation (3.1) can be decoupled into a pair of two-dimensional equations, as follows

$$\begin{aligned} -i\hbar c(\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}) \chi &= (E - mc^2 - V) \phi, \\ -i\hbar c(\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}) \phi &= (E + mc^2 - V) \chi, \end{aligned} \quad (3.2)$$

These two equations share exactly the same structure of the second pair of Maxwell's equations in Eq. (A2), via the rough correspondences

$$\hbar \leftrightarrow 1/k_0, \quad \phi, \chi \leftrightarrow \mathbf{E}, \mathbf{H}, \quad V(\mathbf{x}) \leftrightarrow \mu(\mathbf{x}), \epsilon(\mathbf{x}). \quad (3.3)$$

However, it seems that in the Dirac's case there is no counterpart of the first two Maxwell equations (A1). This is one of the main differences between photons and electrons, and implies that the polarization treatment is rather different in both cases, including the lack of non relativistic spin-effects in the general case.

Continuing with the analogy, we construct now a kind of second-order differential wave equation for the Dirac case equivalent to Eq. (A3). This is always possible clearing χ from the second equation of Eq. (3.2) and substituting it into the first one

$$\hbar^2 \nabla^2 \phi + \left[\left(\frac{E - V}{c} \right)^2 - m^2 c^4 \right] \phi + \frac{\hbar^2 \nabla V \cdot \nabla}{E - V + mc^2} \phi + i \frac{\hbar^2 \boldsymbol{\sigma} \cdot [\nabla V \times \nabla]}{E - V + mc^2} \phi = 0. \quad (3.4)$$

lowing result for the order \hbar^0 :

$$[\nabla W(\mathbf{x})]^2 = \left[\frac{E - V(\mathbf{x})}{c} \right]^2 - m^2 c^4. \quad (3.6)$$

This is the analog of an eikonal equation independent of spin for the electron, fully analogous to the Eq. (A5) of the electromagnetic case. Comparing Eqs. (3.6) and (A5), it is very remarkable that the only real difference between them is the fact of the former has mass.

On the other hand, the order \hbar^1 of the previous expansion leads us to

$$\frac{d}{ds} \phi_0 = -\frac{\nabla^2 W}{2|\nabla W|} \phi_0 - \frac{(\nabla V \cdot \boldsymbol{\sigma})(\nabla W \cdot \boldsymbol{\sigma})}{2(E + mc^2 - V)|\nabla W|} \phi_0, \quad (3.7)$$

that after relation (2.8) is equivalent to

$$\frac{d}{ds} \phi_0 = -\frac{\nabla^2 W}{2|\nabla W|} \phi_0 - \frac{\nabla V \cdot \nabla W}{2(E + mc^2 - V)|\nabla W|} \phi_0 - i \frac{(\nabla V \times \nabla W) \cdot \boldsymbol{\sigma}}{2(E + mc^2 - V)|\nabla W|} \phi_0, \quad (3.8)$$

being

$$\frac{d}{ds} = \frac{\nabla W \cdot \nabla}{|\nabla W|} \quad (3.9)$$

the derivation along the arc length of the trajectory.

This is precisely transport equation we were looking for. As we announced, it shares exactly the same structure of the electromagnetic counterpart in Eq. (A6) since both are linear equations of the form $d\mathbf{A}/ds = M\mathbf{A}$. The type of algebra in each case is, however, different. In the Maxwell transport, the vectorial field itself is coupled with the gradient of inhomogeneous parameters and with the trajectories. Dirac transport, on the other hand, couples vectorially the trajectories, the gradient of the scalar potential and the spin, but now the field has a spinorial character and due to its tensorial properties it cannot be specifically coupled with the dynamical variables, which are vectors. This is the last important difference we have found between photons and electrons. A further development will show how these characteristics of Eq. (3.8) imply some geometrical consequences in the transport of the 1/2-spin particle.

Note that in the non relativistic limit $E - mc^2 \ll mc^2$ the spin-trajectory coupling between $\boldsymbol{\sigma}$ and ∇W disappears. Thus spin transport in the absence of magnetic fields is a purely relativistic phenomenon.

B. Amplitude and spin

The general transport equation (3.8) can be split into equations for amplitude $|\phi_0|$ and local spin state \mathbf{u}_0 , both depending on \mathbf{x} , after decomposing ϕ in the form

$$\phi_0 = |\phi_0|\mathbf{u}_0, \quad |\mathbf{u}_0| = 1. \quad (3.10)$$

For the amplitude $|\phi_0|$ we get

$$\frac{d}{ds}|\phi_0| = - \left(\frac{\nabla^2 W}{2|\nabla W|} + \frac{\nabla V \cdot \nabla W}{2(E + mc^2 - V)|\nabla W|} \right) |\phi_0|, \quad (3.11)$$

while for the spin state \mathbf{u}_0 we have

$$\frac{d}{ds}\mathbf{u}_0 = -i \frac{(\nabla V \times \nabla W) \cdot \boldsymbol{\sigma}}{2(E + mc^2 - V)|\nabla W|} \mathbf{u}_0. \quad (3.12)$$

In particular this last expression allow us to derive a transport equation for the local mean value $\langle A \rangle$ of any spin observable A as

$$\langle A \rangle = \mathbf{u}_0^\dagger A \mathbf{u}_0, \quad \frac{d}{ds}\langle A \rangle \propto -i\langle [\mathbf{b}' \cdot \boldsymbol{\sigma}, A] \rangle, \quad (3.13)$$

and in particular

$$\frac{d}{ds}\langle \boldsymbol{\sigma} \rangle \propto \langle \boldsymbol{\sigma} \rangle \times \mathbf{b}', \quad (3.14)$$

where here $\mathbf{b}' \propto \nabla V \times \nabla W$, and by local we mean that $\langle A \rangle$ depends on \mathbf{x} . This is that the spin transport is

made of consecutive local rotations around the vector \mathbf{b}' . In particular, the projection of the spin on the vector \mathbf{b}' is constant $\langle \mathbf{b}' \cdot \boldsymbol{\sigma} \rangle = \text{constant}$.

We can particularize to the harmonic oscillator $V(\mathbf{x}) \propto \mathbf{x}^2$ comparing with the result for the Dirac oscillator above. In such a case the trajectories are in the plane defined by ∇V and ∇W so that $\mathbf{b}' \propto \mathbf{b}$. Nevertheless, in this case the spin state needs not be constant and its evolution will depend in general of the trajectory followed. Moreover, the transport equation depends on dynamical features other than the form of the trajectory, so seemingly also in this case the geometrical character of the transport is lost in the transition from light to matter.

IV. CONCLUSIONS

For scalar wave-functions it is known that the discontinuities propagate following classical trajectories, in the same way that the discontinuities of the electromagnetic field follow geometrical light rays. We have examined the propagation of spin discontinuities for a 1/2-spin particle obeying Dirac equations with scalar potentials. We have fully achieved this goal for the case of the Dirac oscillator showing a definite relation between the spin discontinuity and the tangent to the classical trajectory.

For situations other than the Dirac oscillator we have established as many clear parallels as possible with the equivalent situation for the electromagnetic field. To this end we have followed an eikonal asymptotic approach after the wave equation. The comparison between the Dirac and Maxwell approaches reveals three main differences: (i) the electromagnetic field satisfies orthogonality relations (A1) that are absent in the Dirac case, (ii) there is a mass term difference in the Dirac eikonal (3.6) in comparison with the Maxwell case (A5), (iii) in the Dirac case there is no projection of spin along the tangent to the trajectory in Eq. (3.12) at difference with the Maxwell case (A12). These differences might explain the lack of spin-propagation effects in the non relativistic limit, and the lack of topological features.

Appendix A: Eikonal approach for the electromagnetic field

We review here the eikonal approach for electromagnetic field to be compared with the Dirac case. The Maxwell's field equations for time-harmonic waves of frequency ω within isotropic and inhomogeneous media are

$$\nabla [\epsilon(\mathbf{x})\mathbf{E}(\mathbf{x}, t)] = 0, \quad \nabla [\mu(\mathbf{x})\mathbf{H}(\mathbf{x}, t)] = 0, \quad (A1)$$

$$-\frac{i}{k_0}\nabla \times \mathbf{E}(\mathbf{x}, t) = \mu(\mathbf{x})c\mathbf{H}(\mathbf{x}, t),$$

$$\frac{i}{k_0}\nabla \times \mathbf{H}(\mathbf{x}, t) = \epsilon(\mathbf{x})c\mathbf{E}(\mathbf{x}, t), \quad (A2)$$

where $k_0 = \omega/c$. They can be combined to get the vectorial wave equation:

$$\nabla^2 \mathbf{E} + n^2 k_0^2 \mathbf{E} + \nabla \left(\frac{1}{\epsilon} \nabla \epsilon \cdot \mathbf{E} \right) + \frac{1}{\mu} \nabla \mu \times (\nabla \times \mathbf{E}) = 0, \quad (\text{A3})$$

where $n(\mathbf{x}) = c\sqrt{\epsilon(\mathbf{x})\mu(\mathbf{x})}$ is the refraction index.

To apply the eikonal approximation in the limit $1/k_0 \rightarrow 0$ we consider asymptotic solutions of the form [2]

$$\mathbf{E} = \left(\mathbf{E}_0 + \frac{1}{k_0} \mathbf{E}_1 + \dots \right) e^{ik_0 S'}, \quad (\text{A4})$$

where $S'(\mathbf{x}, t) = L(\mathbf{x}) - ct$ is the phase. Introducing Eq. (A4) into Eq. (A3) we get for the lowest $1/k_0^0$ order

$$[\nabla L(\mathbf{x})]^2 = n^2(\mathbf{x}), \quad (\text{A5})$$

which is the well known eikonal equation.

For the $1/k_0^1$ order we have

$$\frac{d}{ds} \mathbf{E}_0 = -\frac{\nabla^2 L}{2|\nabla L|} \mathbf{E}_0 - \frac{(\mathbf{E}_0 \cdot \nabla \epsilon) \nabla L}{2\epsilon|\nabla L|} - \frac{\nabla \mu \times (\nabla L \times \mathbf{E}_0)}{2\mu|\nabla L|}, \quad (\text{A6})$$

where

$$\frac{d}{ds} = \frac{\nabla L \cdot \nabla}{|\nabla L|}, \quad (\text{A7})$$

is the derivation with respect the arc length s . The last term in Eq. (A6) can be expressed also as

$$\frac{\nabla \mu \times (\nabla L \times \mathbf{E}_0)}{2\mu|\nabla L|} = \frac{(\mathbf{E}_0 \cdot \nabla \mu) \nabla L}{2\mu|\nabla L|} - \frac{(\nabla L \cdot \nabla \mu) \mathbf{E}_0}{2\mu|\nabla L|}. \quad (\text{A8})$$

This is the transport equation that expresses the propagation of amplitude and polarization of the photon along the trajectories determined by the eikonal equation (A5).

On the other hand, if we insert Eq. (A4) directly in Eq. (A1) we get again Eq. (A5) plus the explicit relations of orthogonality

$$\mathbf{E}_0 \cdot \nabla L = 0, \quad \mathbf{H}_0 \cdot \nabla L = 0. \quad (\text{A9})$$

The transport equation (A6) can be further split into propagation equations for the local amplitude $|\mathbf{E}_0|$ and the local polarization state \mathbf{u}_0 , both depending on \mathbf{x} , after decomposing \mathbf{E}_0 in the form

$$\mathbf{E}_0 = |\mathbf{E}_0| \mathbf{u}_0, \quad |\mathbf{u}_0| = 1. \quad (\text{A10})$$

This leads to the following equation of propagation for the local amplitude $|\mathbf{E}_0|$

$$\frac{d}{ds} |\mathbf{E}_0| = - \left(\frac{\nabla^2 L}{2|\nabla L|} - \frac{\nabla L \cdot \nabla \mu}{2\mu|\nabla L|} \right) |\mathbf{E}_0|, \quad (\text{A11})$$

and to this one for the local polarization state \mathbf{u}_0

$$\frac{d}{ds} \mathbf{u}_0 = - \frac{(\mathbf{u}_0 \cdot \nabla \epsilon) \nabla L}{2\epsilon|\nabla L|} - \frac{(\mathbf{u}_0 \cdot \nabla \mu) \nabla L}{2\mu|\nabla L|}. \quad (\text{A12})$$

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